

Crystallization of the resonating valence bond liquid as vortex condensation

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We show that the liquid-to-crystal quantum phase transition in the Rokhsar–Kivelson dimer model on the two-dimensional triangular lattice occurs as a condensation of vortex-like excitations called “visons”. This conclusion is drawn from the numerical studies of the vison spectrum in the liquid phase by using the Green’s function Monte Carlo method. We find that visons remain the lowest excitation throughout the liquid phase and that their gap decreases continuously to zero at the phase transition. The nature of the crystal phase and the second order of the phase transition are in agreement with the earlier prediction of Moessner and Sondhi [Phys. Rev. B **63**, 224401 (2001)].

The resonating valence bond (RVB) liquid is one of the most intriguing concepts of today’s condensed-matter physics. Conjectured over thirty years ago for frustrated spin systems, [1] it still lacks an adequate quantitative description, and even its emergence in real physical materials or in realistic spin models is not rigorously established. In the early days of the RVB paradigm, it has been realized that such a state should be characterized by a Z_2 topological order whose most prominent consequence is the vortex-like excitation [2] later dubbed “vison”. [3] This type of excitations should be important for the thermodynamics of RVB spin liquids and serve as a “smoking gun” of the RVB phase. Numerically, low-lying singlet excitations have been found in the Kagome spin-1/2 Heisenberg antiferromagnet, [4] the most promising candidate for the RVB spin-liquid state, and these singlets have been interpreted as RVB states in the subspace of nearest-neighbor singlet dimers. [5] Experimentally, the spin-1/2 Kagome system with a possible spin-liquid phase has been realized recently in the $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ compound. [6] A variational study of this system with Gutzwiller-projected wave functions also predicts low-lying excitations of the gauge field [$U(1)$ instead of Z_2]. [7] Thus the properties of the low-lying collective singlet excitations is one of the central questions in the study of RVB states.

To model the vison branch of excitations in the RVB state, it has been proposed to use dimer models instead of spin ones. [8] In dimer models, the spin degrees of freedom are explicitly frozen, and only the vison excitations survive. Regardless of its relation to microscopic spin models, the quantum dimer model (QDM) of Rokhsar and Kivelson (RK) has attracted a lot of attention as a promising way to investigate RVB physics, especially on the triangular lattice. The QDM is defined by:

$$H = -t \sum \left(| \diagup \diagdown \rangle \langle \text{---} | + h.c. \right) + V \sum \left(| \diagup \diagdown \rangle \langle \diagup \diagdown | + | \text{---} \rangle \langle \text{---} | \right), \quad (1)$$

where the sum runs over all plaquettes (rhombi) including the three possible orientations. The kinetic term controlled by the amplitude t flips the two dimers on every flippable plaquette, i.e., on every plaquette with two parallel dimers, while the potential term controlled by the interaction V describes a repulsion ($V > 0$) or an attraction ($V < 0$) between nearest-neighbor dimers. For dimer models, the situation is much more definite than for spin systems: The RVB phase is firmly established and studied in detail in the QDM on the triangular lattice. [9] At the special so-called RK point in the parameter space ($V = t$), an analytic proof of the topological degeneracy is possible. [10, 11] At the same RK point, the quantum-mechanical evolution in imaginary time is equivalent to a classical stochastic process which allows to deduce the quantum excitation gap from a *classical* Monte Carlo study. [12] With such a numerical work, it has been established that the elementary excitations are indeed visons, that is the gap in the vison excitation sector (non-local in terms of dimers) is lower than that in the dimer sector. [13] Dimer excitations are then interpreted as composite two-vison states.

With the Green’s function Monte Carlo (GFMC) method, [14, 15] we can extend this approach away from the RK point $V = t$ to a wider class of systems (provided the ground state is positive definite, i.e., for models without the sign problem). In application to the QDM, this method allows us to study the boundaries of the RVB phase and the transitions to the crystal phases. In our earlier works, [16, 17] we have computed the static and dynamic dimer correlations in the QDM for different values of V/t . Based on those results, we have refined the phase diagram proposed by Moessner and Sondhi on the basis of the quantum Monte Carlo studies (at finite temperature). [9] We have found a crystal phase with a 12-site unit cell (as predicted in Refs. 9, 18) which destroys the RVB phase at the critical parameter value $V/t \approx 0.8$. At the transition point, the static form factor of the crystal decreases to zero on the crystal side of the transition, while the dimer gap also decreases to zero on the liquid

side. [17]

However, an interesting question remains about the fate of visons at this phase transition. Firstly, visons are expected to be more fundamental excitations than dimers, at least at the RK point. [13] Secondly, to describe this phase transition, Moessner and Sondhi used the mapping of the RK dimer model at $V = 0$ onto the frustrated Ising model on the dual (hexagonal) lattice with a weak transverse field. [18] In this mapping, the spins of the Ising model correspond to the visons of the dimer model and the crystallization transition was described as the ordering of Ising spins equivalent to the condensation of visons. They have further conjectured that the same type of transition should occur in the dimer model as a function of V/t .

To test this conjecture, we have performed numerical studies of the dynamic and static vison correlation functions with the use of the GFMC method. We find that as the parameter V/t of the QDM decreases below the RK point, the vison gap gradually decreases and reaches zero at the presumed crystallization point. On the other side of the transition, the Bragg peaks in the static vison correlations gradually appear signaling the crystal phase. This numerical evidence of the crystallization transition by vison condensation is the main result of our work.

Visons.— Vison operators and corresponding excitations in QDM have been constructed and considered in detail in Refs. 2, 3, 13. Here we briefly recall the main principles of the construction.

Point-vison operators are defined on the sites of the dual lattice (in our case, on the triangular plaquettes forming a honeycomb lattice). In a closed system (without open boundaries), only products of even number of visons are well defined. The product of two point visons is defined by

$$V_i V_j = (-1)^{\text{no. of dimers intersecting } \Gamma_{ij}} \quad (2)$$

where Γ_{ij} is some path on the dual lattice connecting the triangular plaquettes i and j . With this definition, $V_i V_j$ is independent of the path Γ_{ij} up to a global sign (the same for all dimer coverings). Even though only products of even number of visons are defined in this way, one can separate the visons far apart in a large system and consider them as individual vortex-like excitations. [2, 3] Moreover, it has been shown in Ref. 13 that in a finite closed system one can also define a product of vison operators taken at different times and hence the correlation function

$$F(\mathbf{r}_{ij}, t - t') = \langle V_i(t) V_j(t') \rangle. \quad (3)$$

The construction is based on inserting the identity operator $V_i(t') V_i(t')$ in the product $V_i(t) V_j(t')$. Then the resulting product of four vison operators may be decoupled into the equal-time product $V_i(t') V_j(t')$ defined by (2) and the equal-position product $V_i(t) V_i(t')$ which simply

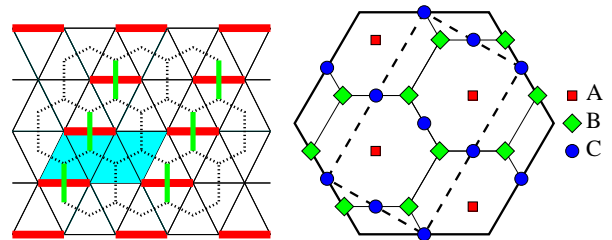


FIG. 1: (Color online) Left panel: The reference dimer configuration for fixing the vison gauge. Dashed black (solid green) lines indicate positive (negative) hoppings for visons on the dual lattice, due to the flux π per hexagonal plaquette. The shaded region is the unit cell for the vison operator (four sites of the dual lattice). Right panel: Brillouin zones for dimers and visons. The Brillouin zone of the triangular lattice is the largest hexagon; the dashed rectangle denotes the Brillouin zone of the vison-like sector. A, B and C denote the high-symmetry points.

counts the number of flips between t and t' on the rhombi containing i . [13]

Remarkably, the asymptotic behavior of the correlation function (3) at large imaginary time gives us access to the gap in the excitation spectrum for a *single* vison, even though the computation is performed for a finite system.

One subtlety in the vison definition is the necessity of the gauge fixing and, as a consequence, an artificial doubling of the unit cell for the correlation function (3). The sign in the vison definition (2) may be fixed by choosing the contour Γ_{ij} for every point i and a reference point j . If the contour Γ_{ij} is deformed to loop around one site of the lattice, the sign of $V_i V_j$ is reversed, since there is exactly one dimer starting from that site. As a result, under the lattice translations, the vison operators V_i transform as particles moving in a magnetic field with the flux π per (hexagonal) plaquette of the dual lattice. A convenient way to fix a gauge for vison operators is to multiply the product of visons (2) by its value in a reference dimer configuration. In terms of the gauge field on the dual (hexagonal) lattice, a choice of the reference configuration translates into assigning the gauge phase factors of -1 to all links intersecting the dimers of the reference configuration. The most symmetric choice of the reference dimer covering is periodic with two sites of the original triangular lattice per unit cell, implying that the unit cell in the dual lattice contains four sites. Such a reference covering is shown in Fig. 1 (left panel). This gauge choice was used in Ref. 13, and the corresponding Brillouin zone for vison excitations is shown in the right panel of Fig. 1. The high-symmetry points of the vison Brillouin zone are labeled A, B, and C.

Numerical method.— The numerical investigations are based on the Green's function Monte Carlo method at zero temperature, [14] adapted to the quantum dimer problem [16, 17]. With the above prescription, the

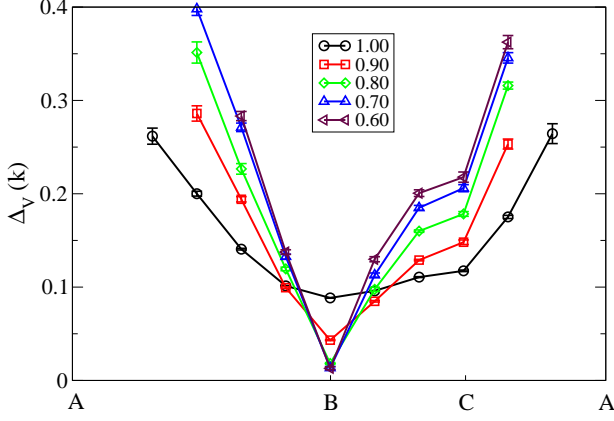


FIG. 2: (Color online) Lowest-energy excitation spectra for the 432-site cluster for different values of V/t .

ground-state vison-vison correlation function in imaginary time $F(\mathbf{r}_{ij}, \tau)$ can be calculated in the same way as the dimer one. [17] Note that since the unit cell of the vison operator contains four dual-lattice sites, the Fourier transform $F(\mathbf{k}, \tau)$ is a 4×4 matrix for each \mathbf{k} point. Since we are interested in the transition between the disordered RVB phase and the $\sqrt{12} \times \sqrt{12}$ crystal, we work only with clusters defined by factorization of the infinite triangular lattice by the translations $\mathbf{T}_1 = l\mathbf{u}_1 + l\mathbf{u}_2$ and $\mathbf{T}_2 = -l\mathbf{u}_1 + 2l\mathbf{u}_2$. Here $\mathbf{u}_1 = (1, 0)$ and $\mathbf{u}_2 = (1/2, \sqrt{3}/2)$ are the unitary vectors defining the triangular lattice and l is an even integer. [19] Such clusters contain $N = 3l^2$ sites and can accommodate the $\sqrt{12} \times \sqrt{12}$ crystal structure without defects. In the present work we study numerically clusters up to $l = 12$.

Vison gap.— The vison gap $\Delta_V(\mathbf{k})$, i.e., the energy of the lowest excitation with the wave vector \mathbf{k} , can be extracted from the long-time behavior of $F(\mathbf{k}, \tau)$. [20] The results for various values of V/t obtained on the $3 \times 12 \times 12$ -site cluster are depicted in Fig. 2. At the RK point, the dispersion reproduces the results of Ref. 13. As V/t decreases below one, the shallow minimum at point B deepens, and the gap gradually closes. To find the value of the vison gap in the thermodynamic limit, we have performed a finite-size analysis of $\Delta_V(B)$ shown in Fig. 3 (left panel). We find that $\Delta_V(B)$ extrapolates to a finite value for $V/t \geq 0.85$ and to zero for $V/t \leq 0.8$.

Similarly to the analysis of the dimer ordering in Ref. 17, we have also calculated the intensity of the static vison Bragg peak at the point B . The size-scaling extrapolation for the Bragg-peak intensity is shown in Fig. 3 (right panel). Near the transition point, the dependence of the Fourier component of the vison correlation on the system size is noticeably nonlinear, and the extrapolation has a low precision. This can be explained by the divergent vison correlation length at the transition point. We can estimate the vison correlation length by extrapolating our data in Fig. 7 in Ref. 16 to the approximate transition point. Such an estimate shows that within the window $(V/t)_c \pm 0.02$ around the transition point, the correlation length is of the order or larger than the largest system size considered in the present work (i.e., $N^{1/2} \sim 20$). Therefore, our results on the Bragg-peak intensities necessarily lack precision within this window around the transition point.

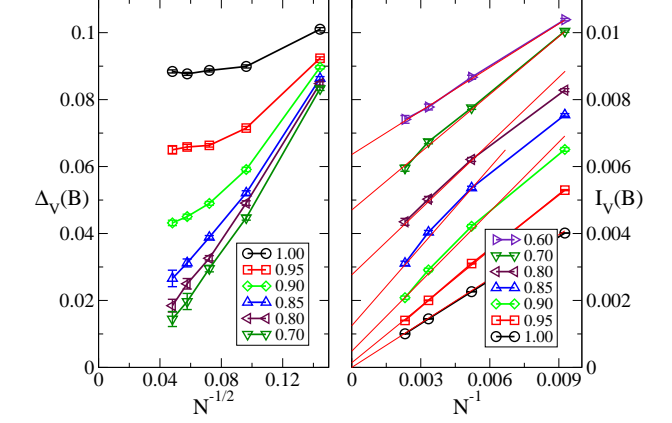


FIG. 3: (Color online) Left: Size dependence of the vison gap at point B . The gap closes at a transition point between $V/t = 0.8$ and $V/t = 0.85$. Right: Extrapolation of the Bragg-peak intensity of the vison at point B to the thermodynamic limit.

We summarize our results on the vison gap and Bragg peaks in Fig. 4, together with our previous data for dimer excitations from Ref. 17. All those data indicate that both vison and dimer excitations close the gap at the transition point, on the liquid side. On the crystal side, the Bragg-peak intensity vanishes continuously, for both dimer and vison correlations. The dimer and vison data are consistent with each other in locating the transition point, which may be estimated as $V/t = 0.83 \pm 0.02$.

Everywhere in the liquid phase, down to the transition point, the lowest vison excitation is always below the dimer gap, which proves that visons are indeed the elementary excitations and allows us to interpret the transition as a *vison condensation*. What is intriguing though in this respect is the relative magnitudes of the vison gap and of the dimer gap reported in Ref. 17. In the dimer sector, the lowest excitation should be at most twice the vison gap (it could be smaller if there is a bound state). Indeed, the dimer-density operator n_{ij} on the bond between two neighboring triangular plaquettes i and j (which gives 1 when applied to a configuration if this bond is occupied by a dimer and 0 otherwise) can be written in terms of the vison operators at plaquettes i and j as

$$n_{ij} = \frac{1}{2}(1 - V_i V_j) \quad (4)$$

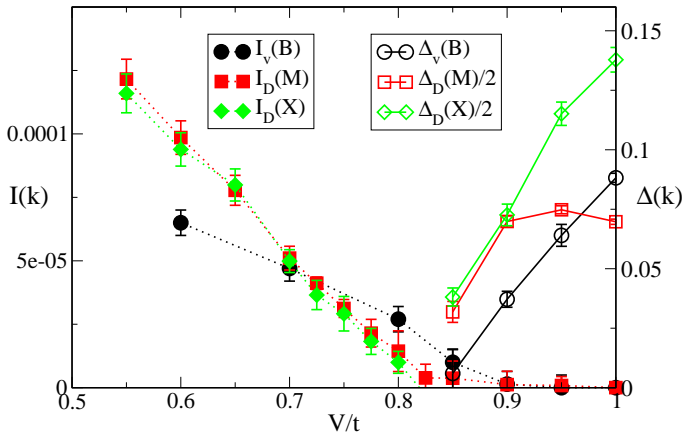


FIG. 4: (Color online) Dimer gaps at point X and M , vison gap at point B , and the corresponding Bragg peaks as a function of V/t . The vison Bragg peaks are multiplied by 0.01. The dimer gaps are divided by 2.

and thus corresponds to two-vison excitations (since point visons do not produce exact eigenstates, dimer operators also generate higher excitations with even numbers of visons). However, at point X , the energy of the dimer excitation reported in Ref. 17 is always larger than twice the vison gap. The same is true at point M for $V/t < 0.97$. To resolve this apparent inconsistency, we have calculated at the RK point ($V/t = 1$) the dynamics of the product of two visons separated by a distance \mathbf{R} larger than one lattice spacing. The energy of such a composite excitation is extracted from the correlation function $\langle V_i(\tau)V_{i+\mathbf{R}}(\tau)V_j(0)V_{j+\mathbf{R}}(0) \rangle$. Interestingly, the obtained gap at point X *decreases* upon increasing \mathbf{R} , while at point M the dependence on \mathbf{R} is the opposite. Both those gaps approach $2\Delta_v(B)$ at large \mathbf{R} .

This suggests the following interpretation: Except close to the RK point ($V/t = 1$) and around the M point, where they form a bound state, visons repel, and, therefore, the matrix element of the dimer operator between the ground state and the lowest state in the two-vison continuum is extremely small. Due to this vison repulsion, we are not able to detect the bottom of the two-vison continuum from the dimer-dimer correlations. This interpretation further suggests that the energy detected with the dimer-dimer correlations in Ref. 17 corresponds not to an eigenstate, but to a *resonance* inside the two-vison continuum whose lower edge is twice the vison gap.

Summary.— By using the GFMC method, we have numerically studied the quantum phase transition from the RVB liquid to a crystal phase in the Rokhsar–Kivelson dimer model on the triangular lattice. Our results indicate a second-order phase transition consistent with the conjecture of Moessner and Sondhi based on a relation to a frustrated Ising model. [18] At the crystallization transition, the vison excitation becomes gapless, and in the crystal phase the vison operator acquires a finite ex-

pectation value. In this respect, it may be suitable to call this crystal order a “vison crystal”, since it has a long-range vison correlation $\langle V_i V_j \rangle$.

These results definitely establish visons as the relevant excitations to describe the transition between a valence-bond solid and a resonating valence-bond liquid. This calls for further investigation of several aspects of their physics, such as the nature of their mutual interaction and the formation of bound states. In that respect, it would be extremely useful to come up with a simple analytical approach, like the Holstein-Primakoff bosonic description of spin waves. A possibility might be to build further on the relationship to the frustrated Ising model in a transverse field. Work is in progress along these lines.

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